

Realizing Thermalization Via an Exact Simulation of a Finite Quantum Bath

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We demonstrate the thermalization of a small but arbitrary quantum system by exactly simulating the unitary evolution of the system and a much larger but finite system (a “bath”) to which it is coupled. While the universe, consisting of the system and bath, remains in a pure state, and undergoes a reversible evolution, the system equilibrates to the Boltzmann distribution. In this general canonical setting, we further show that the underlying mechanism for the relaxation is that of “eigenstate-thermalization”.

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In the last few years considerable progress has been made in understanding how thermodynamical behavior emerges from quantum mechanics. This fundamental question has been approached from a number of different directions. Recent results have shown that if a quantum system is large enough, almost all states will be “typical”, and have properties that are close to those of micro-canonical averages [1, 2]. Naturally, such micro-canonical averages become the canonical (Boltzmann) distribution when the universe is decomposed into a system and bath. Further, it has been shown rigorously, and under fairly weak conditions, that large systems will induce effectively irreversible behavior in small subsystems [3–5], and very recently that system-bath interactions with random phases will induce thermalization in small systems [6]. From another direction, it has recently been demonstrated via an explicit simulation that a many-body system will thermalize to the micro-canonical ensemble [7]. (That is, the values of single-particle observables are those predicted by the micro-canonical ensemble.) This work also revealed that in this many-body system, the thermalization was a result of the fact that almost every energy eigenstate of the full system gives the micro-canonical values for single-particle observables. That is, the thermalization happens at the level of the individual eigenstates. This phenomena was termed “eigenstate-thermalization” when it was conjectured by Srednicki in 1994 [8], and also has its origins in the work of Shnirelman [9] and Deutsch [10]. Various other authors have contributed to this line of work [11–14], and it is further connected to Berry’s conjecture [15]. In fact, the recent work on typicality by Popescu *et al.* [1] and Goldstein *et al.* [2] also makes eigenstate thermalization plausible — all thing being equal, one would expect the eigenstates of a system to be typical states.

While the numerical results of Rigol *et al.* [7] demonstrated micro-canonical thermalization for a many-body system, they did not give canonical thermalization. For another many-body example, canonical thermalization was indicated to some extent in the simulation by Skrøvseth [16], although the results varied significantly with the initial state of the system. Our goal here is to

demonstrate the canonical (Boltzmann) thermalization of an arbitrary quantum system by a fixed large quantum system (a quantum thermal bath) to which it is coupled. Note that in doing so, the temperature must be fixed by the properties of the bath alone. We are motivated not only by the question of whether this can be achieved with feasibly-sized baths, but because the ability to do so would open a new avenue for exploring the origin of thermal behavior in quantum systems. In particular, in our work here we are able to show that eigenstate thermalization plays a central role in this very generic setting. We also expect that these methods will provide a feasible way to explore the dynamics of strongly damped nonlinear systems, for which approximate master equation techniques, the usual workhorse of open-systems theory, break down [17, 18].

The Hamiltonian of our universe is given by

$$H_{\text{unv}} = H_{\text{sys}} + \hbar g X^{\text{sys}} \otimes Y^{\text{bath}} + H_{\text{bath}}, \quad (1)$$

where H_{sys} is the system Hamiltonian, H_{bath} is the bath Hamiltonian, X^{sys} is the system coupling operator, Y^{bath} is the bath coupling operator, and g is a constant setting the overall size of the coupling. In what follows we always work in the joint energy-eigenbasis of the system and bath, so that H_{sys} and H_{bath} are diagonal.

Since the bath must thermalize any system, it is the properties of the bath, along with those of Y^{bath} , that are the key to obtaining thermal behavior. The properties of our bath are as follows:

- 1) The bath must be chosen to have a density of energy eigenstates that increases exponentially with energy. This condition is essentially just the usual equilibrium thermodynamic assumption — the Boltzmann distribution for a small system in contact with a bath results directly from the assumptions that 1) the density of states of the bath is exponential as a function of energy, 2) that the energy of the universe is conserved, and 3) that all states of the universe are equally likely. The temperature of the bath is given by $T = 1/(k_B \beta)$, where the energy-density of states is $D(E) \propto \exp(\beta E)$. By definition, the temperature of a thermal bath should not change as energy is added (the bath is “big”), which means merely that β is a constant, independent of E .

2) The bath must have a large enough energy range that in interacting with the bath, the system can make energy-conserving transitions between its highest and lowest energy states. For the simulations below, the energy range of our system is $3.5\hbar\mu$, where μ sets the overall energy scale of the simulation. We choose our bath to have 5000 states covering the energy interval $\hbar\mu[3, 20.0465]$, with $\beta = 0.4$.

3) The initial state of the bath must contain a large number of energy eigenstates of the universe, which translates to a large number of energy eigenstates of the bath. We choose the initial state of the bath to be an equal superposition, with random phases, of a set of 350 contiguous bath energy eigenstates spanning the interval $\hbar\mu[12.4, 14.1]$. The initial bath state must be chosen so that all the states of the system are accessible from any initial system-state by exchanging energy with the bath. The appropriate window is most easily selected by examining the eigenstates of the universe Hamiltonian, which we examine further below.

4) The bath interaction operator, Y^{bath} requires some complexity — that is, its elements should, at least locally, vary in a more-or-less random fashion. For example, interaction operators resulting from two-body interactions in a many-body system are typically complex in this manner. This is simplest to achieve by making the off-diagonal elements Gaussian random numbers, with unit variance. We set the diagonal elements of Y^{bath} to zero, so as to minimize their effect on the bath spectrum. We also choose the interaction, along with all other contributions to the universe Hamiltonian, to be real. This reduces the numerical overhead in diagonalizing the Hamiltonian.

5) The typical elements of the interaction operator, $gX^{\text{sys}} \otimes Y^{\text{bath}}$ must be significantly larger than the separation between adjacent bath energy levels. This is crucial, because to generate energy exchange between the system and bath, the interaction must be non-perturbative as far as the universe is concerned. Of course, in order to preserve the energy levels of the system, the interaction $gX^{\text{sys}} \otimes Y^{\text{bath}}$ must be perturbative from the point of view of the system. Note that due to the exponential spectrum of the bath, the bath states at the lower end of the spectrum are necessarily more sparse in energy. To minimize the effect of this sparsity, we increase the overall size of the elements of the bath interaction operator for the low-energy states. While this is not strictly necessary, it keeps the interaction non-perturbative for the low-energy part of the bath spectrum, and thus improves thermalization for low-energy initial states. The precise form of the bath operator we use is as follows. If we denote the bath energy eigenvalues as ε_i (energy increasing with the index i), then the matrix elements Y_{ij}^{bath} are given by

$$Y_{ij}^{\text{bath}} = \left[1 + (\eta/\Delta\varepsilon_0) \sqrt{\Delta\varepsilon_i \Delta\varepsilon_j} \right] w_{ij} \quad (2)$$

where for $i < j$, $\Delta\varepsilon_i = \varepsilon_{i+1} - \varepsilon_i^{\text{bath}}$, $\Delta\varepsilon_j = \varepsilon_j - \varepsilon_{j-1}$, and w_{ij} is a zero mean Gaussian random number with unit variance. Here $\Delta\varepsilon_0$ is the energy gap between the lowest two energy states of the bath, chosen to be $\Delta\varepsilon_0 = \mu \exp(-\beta E_0)$, with E_0 the bath ground state. For our simulations we set $g = 5 \times 10^{-3}\mu$, and $\eta = 100\Delta\varepsilon_0$.

Now we have determined the structure of the bath, it is time to couple it to a small system. To limit the numerical overhead, we use a system with just four states. Naturally, the bath is required to thermalize *any* system, including any system interaction operator X^{sys} , with the only condition that X^{sys} be sufficiently non-commuting with H^{sys} . We therefore make an arbitrary choice for the system energy levels and interaction operator X^{sys} . The energy levels of our the system to be $\hbar\mu[0.5, 1.5, 2.2, 4]$. Denoting the matrix elements of X^{sys} by x_{ij} , we choose $x_{12} = -0.7$, $x_{13} = 0.3$, $x_{14} = -0.9$, $x_{23} = -1.2$, $x_{24} = -0.4 = -x_{34}$. The diagonal elements of X^{sys} are set to zero, since there is no sense in unnecessarily perturbing the system.

To demonstrate thermalization we must evolve the system for an arbitrarily long time. Obtaining an essentially exact evolution for long times can be achieved by performing a full diagonalization of the Hamiltonian of the universe, H^{unv} . Since the Hamiltonian is a (real) 20,000 dimensional matrix, this diagonalization does require a very large RAM. Nevertheless, with currently available computing resources, and absolute addressing, this is now quite feasible. In fact, we have already diagonalized real Hamiltonians that are twice this size, and even larger problems are clearly feasible.

In Fig. 1 we present the results of the simulation, for two initial states of the system, being respectively the lowest and highest energy levels. Both initial states relax as desired to the thermal Boltzmann distribution and remain there, albeit with small fluctuations. Interestingly, when the system starts in its ground state, the residual fluctuations are larger than when it starts in its highest energy state. We will return to this phenomena below, which is due to the finite size of the bath.

We now turn to the question of the eigenstate thermalization hypothesis [7]. If eigenstate thermalization occurs, then for each eigenstate of the universe, the reduced state of the system (that is, traced over the bath) will be the thermal Boltzmann state. We will refer to the population for a system energy eigenstate that results from the universe being in a single energy eigenstate, as the “eigenstate-value” for that population. These “eigenstate-values” are shown in the four plots in Fig. 2. In each of the four plots, the horizontal solid line gives the Boltzmann population for the respective state. The dark (noisy) line gives the eigenstate-values for the population as a function of the energy of the eigenstates. While we see that the eigenstate-values are in fact *not equal* to the thermal value, since they fluctuated significantly, what is striking is that for a broad range of energy in the middle

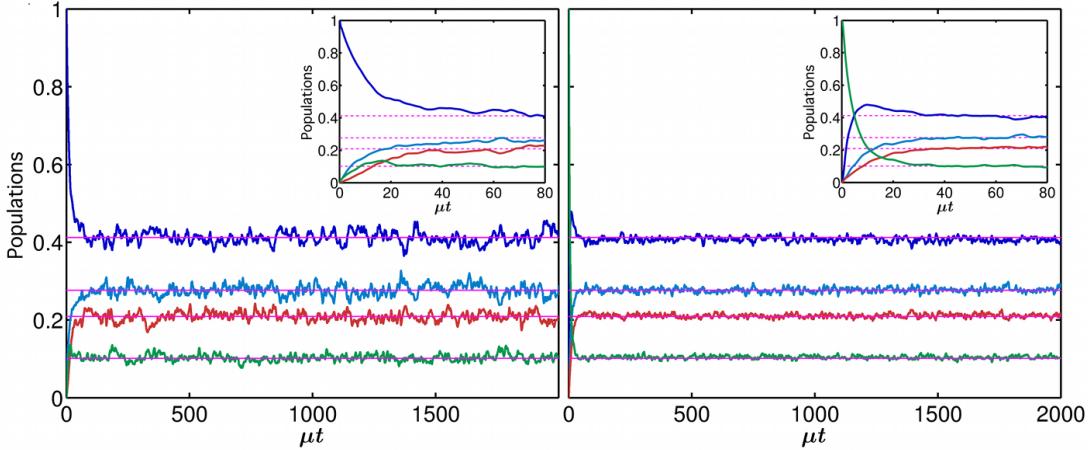


FIG. 1. (Color online) The evolution of the populations of the energy-eigenstates of a nonlinear 4-level system coupled to a bath with 5,000 states, for two initial states of the system. The horizontal lines give the populations for the Boltzmann thermal distribution at the relevant temperature. In plot (a) the initial state is the one with lowest energy, and in (b) it is the state with the highest energy. The insets are expanded versions of the plots for early times, showing the initial relaxation to the thermal state.

of the universe spectrum, the eigenstate values fluctuate randomly about a mean that *is equal* to the thermal value. This is revealed by taking a moving average of the eigenstate-values, and we see that this matches the thermal value over a broad range. As the interaction strength is increased (or alternatively the density of bath states is increased), the fluctuations (deviations) of the eigenstate values from the thermal value decrease. This can be seen in Fig. 2, from the fact that the fluctuations of the eigenstate-values decrease as the eigenstate-energy, and thus the density-of-states, increases. Thus as the size of the bath is increased, the eigenstate-values will tend to the thermal values, with the result being eigenstate-thermalization. Note that it is quite natural that eigenstate-thermalization happens only for a window of energy in the center of the spectrum, and not at the edges. The reason for this is that if the initial state of the bath is on the upper (respectively lower) extreme of its energy range, then the system cannot thermalize because it cannot transfer energy to (respectively from) the bath. The system can only thermalize if the initial state of the bath, and therefore the state of the universe, is not at the edges of its spectrum.

Our results also reveal that complete eigenstate thermalization is *not required* for a bath to succeed in thermalizing an arbitrary quantum system. For our case, the fluctuations of the eigenstate-values about the thermal values are still large, yet the steady-state fluctuations of the *system* about the thermal values are small. This is due to the fact that the initial state of the bath is spread over a large number of adjacent energy eigenstates, and so the steady-state for the system is given by *averaging* over many adjacent universe eigenstates. To achieve thermalization, it is thus only necessary that the average

of a large number of adjacent eigenstate-values correctly gives the thermal value, the individual eigenstate-values can still have large fluctuations.

The above analysis reveals why the steady-state fluctuations of the system are significantly larger when its initial state is the ground state (Fig. 1a) as opposed to the highest energy state (Fig. 1b). This is because we chose the *same* energy window for the bath in both cases. As a result, in the former case, the state of the universe covers a *lower* energy window, a window over which the density-of-states is lower, and the fluctuations of the eigenstate-values are consequently larger. (The distribution of the state of the universe over its energy-eigenstates is shown in the dashed box in first plot in Fig. 2, for the two initial states of the system). Since steady-state fluctuations of the system are due to, and directly proportional to, the fluctuations of the eigenstate-values, these will be larger when the system starts in the ground state. Further, this shows that we *reduce* these fluctuations if we wish, by choosing the initial state of the bath to lie in a higher energy window.

We can also gain insight into *why* the average of the eigenstate-values gives the correct thermal value, independent of the extent to which eigenstate-thermalization is realized. The key is that even with the interaction turned off ($g = 0$), the average of the eigenstate-values equals the thermal value, precisely because the bath has an exponential density of states. All that is required of the interaction operator is to preserve this average, and a random bath interaction operator achieves this.

Important open questions to be explored further concern the class of interaction operators Y^{bath} from which thermal behavior will emerge, and precisely how it is that operators in this class arise from the structure of many-

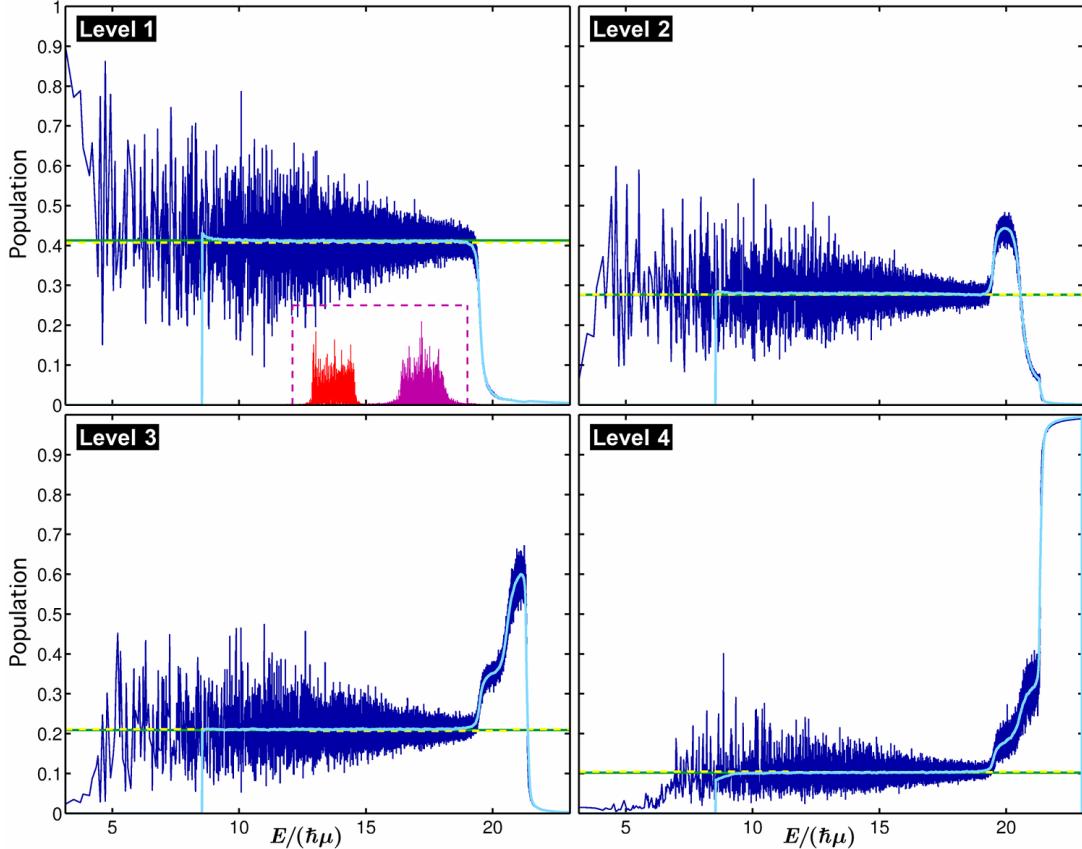


FIG. 2. (Color online) Each of the four plots shows the populations of one of the system energy levels (of which there are four). In each plot: The dashed horizontal line is the desired thermal (Boltzmann) value. The dark noisy line is the population given by each of the energy eigenstates of the universe, as a function of their energy. The solid light grey line is the moving average of the noisy line over a window of 200 adjacent eigenstates. The solid horizontal line is the actual steady-state population when the initial state is state 4. The dashed box in the plot for level 1: the distribution of the initial state of the universe, over its eigenstates, when the system starts in state 1 (left) and 4 (right).

body systems.

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